

The ADDRESS project at the Swiss Light Source: beamline for RIXS studies on novel nano-structure and correlated materials



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Collaborations

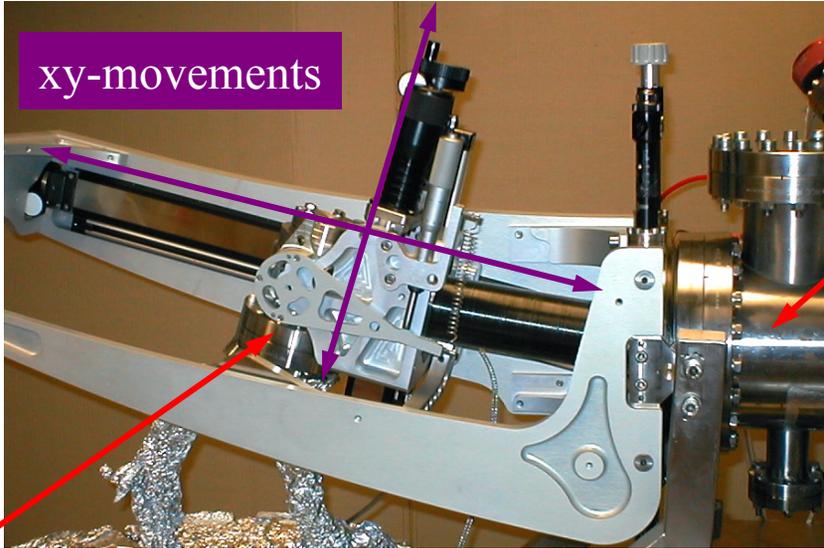
- Vanadium oxides: J. Nordgren, L.-C. Duda, A. Augustsson, M. Mattesini, R. Ahuja (Dept. of Physics, Uppsala Univ.), J.-H. Guo (ALS – LBNL), M. Matsubara (Univ. of Helsinki), A. Kotani (SPring-8), J. Höwing, T. Gustafsson (Uppsala Univ.), M. Klemm, S. Horn, V. Eyert, U. Schwingenschlögl (Univ. of Augsburg), P. Kuiper (Växjö Univ.)
- Ga(In)AsN: V.N. Strocov (SLS) and P.O. Nilsson (Chalmers University of Technology, Gothenburg)



Outline

- Scientific cases: RIXS in vanadium oxides and diluted semiconductors (GaInAsN)
- ADRESS-Project at Swiss Light Source

Experimental set-up



Gratings

Total Fluorescence

Yield detector

Sample

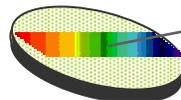


Refocussing optics

Slit

Detector

Soft X-Ray Spectrometer



Imaging detector

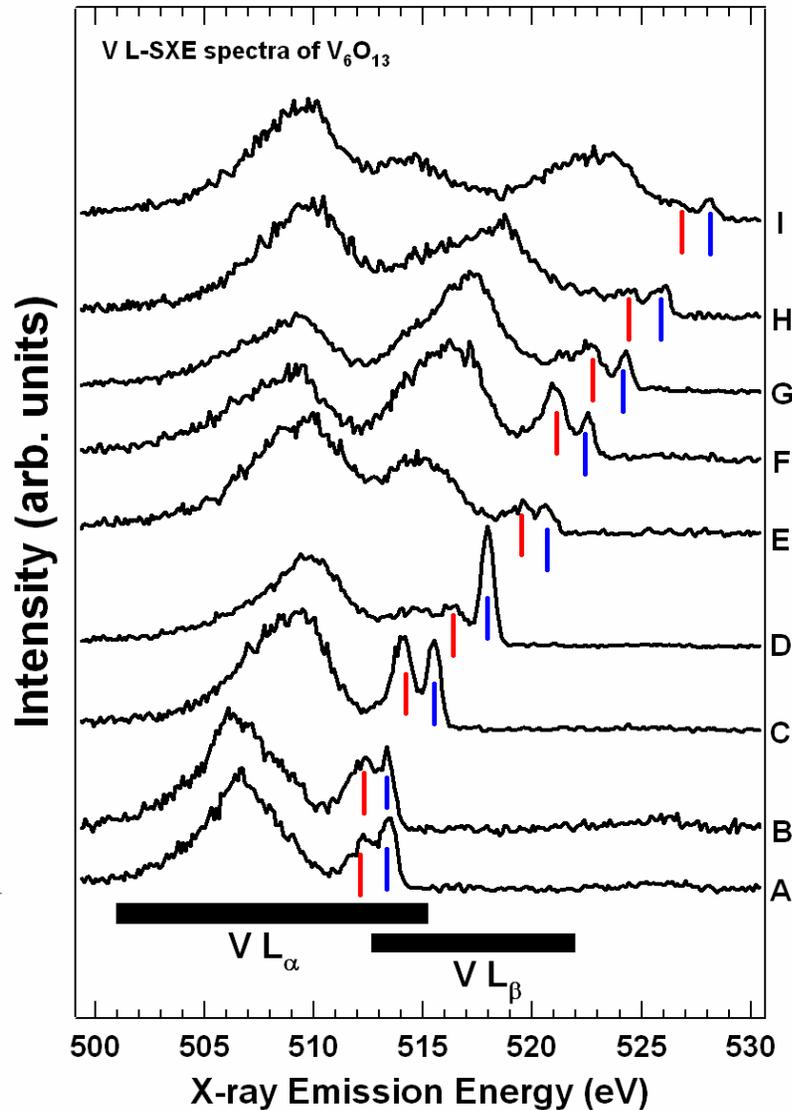
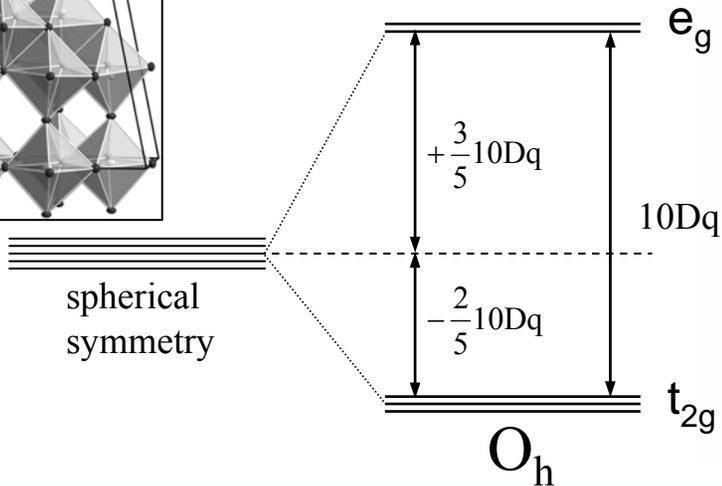
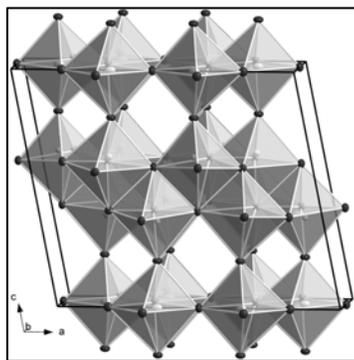
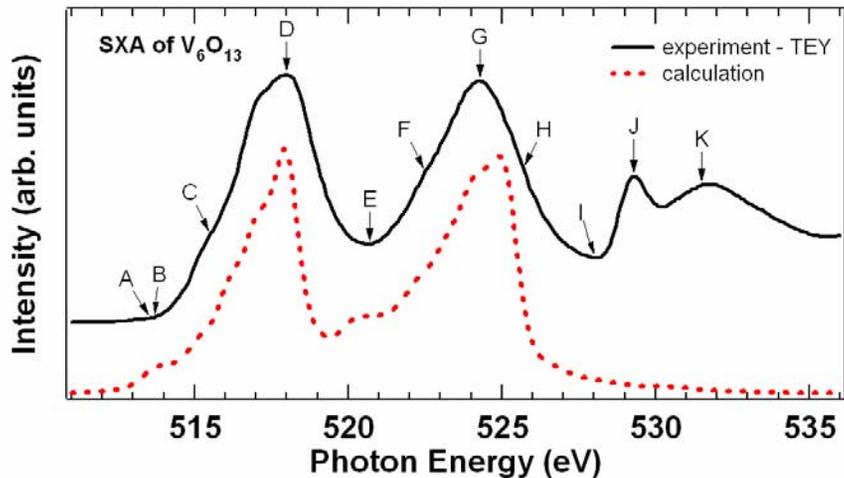
Gratings

Monochromator

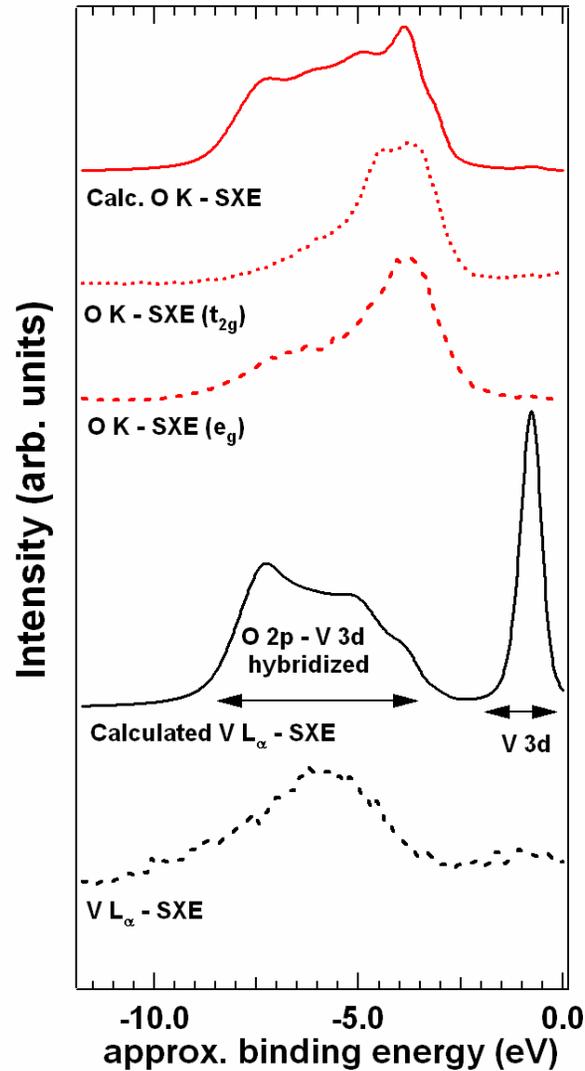
Undulator

e^-

SXA and SXE spectra of V_6O_{13}



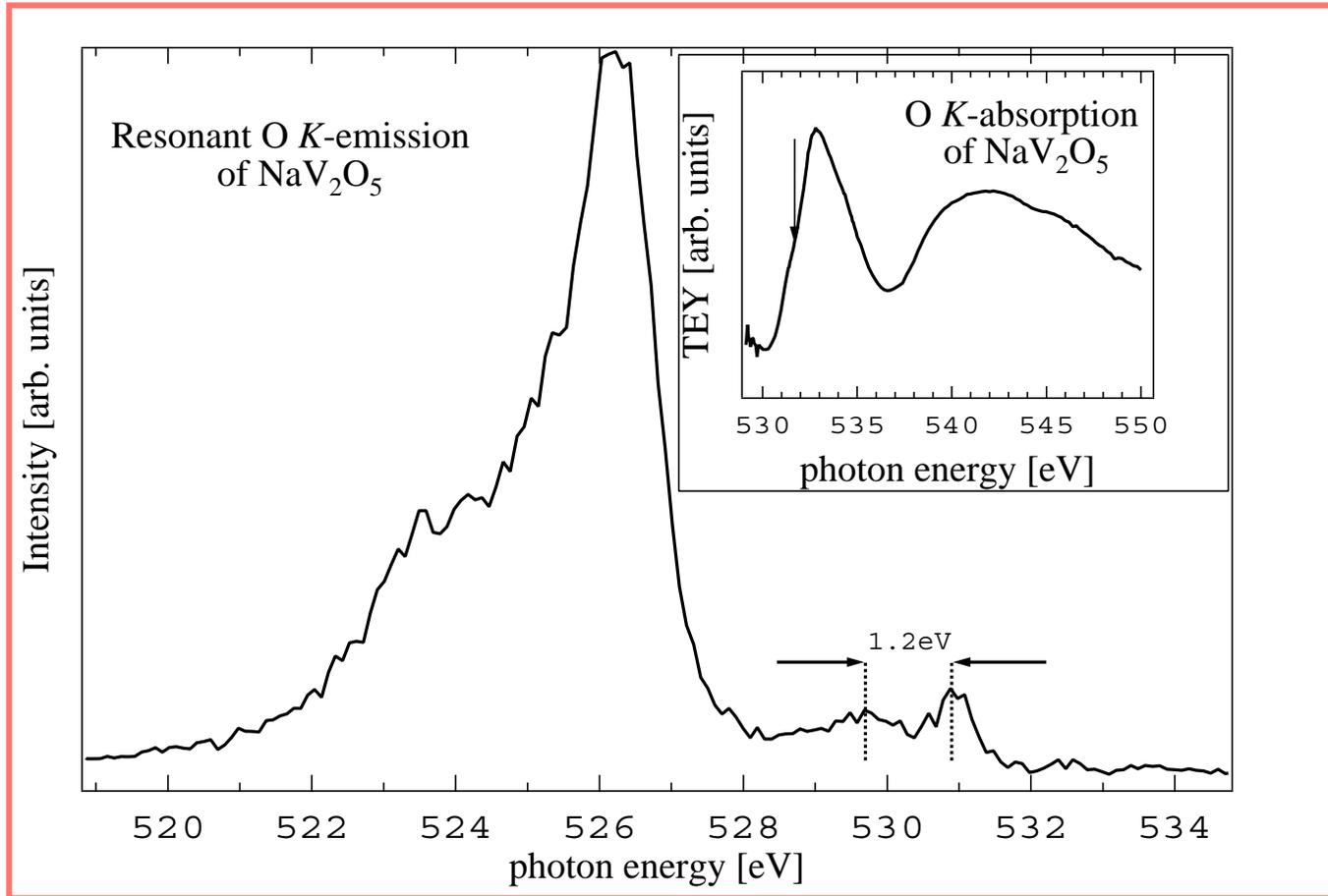
Delocalized picture



**PDOS from
DFT calculations**

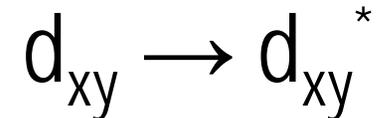
T. Schmitt et al.,
Phys. Rev. B (2004)

O 1s RIXS of NaV₂O₅



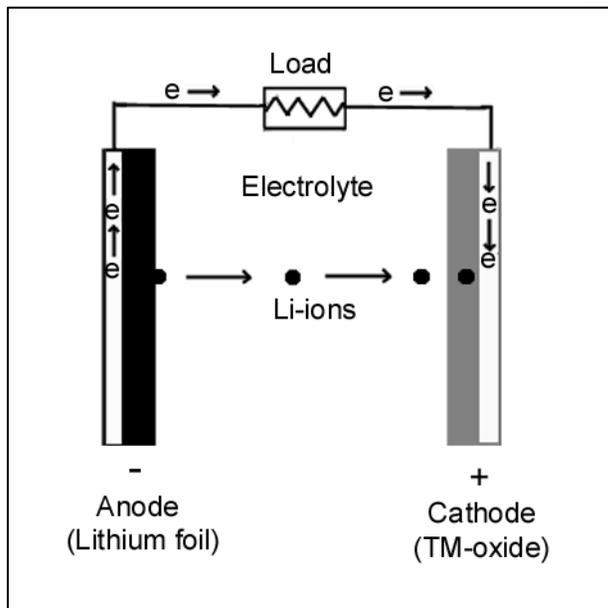
V – O – V rungs

On-rung transitions between bonding and antibonding molecular orbitals with O 1s RIXS:



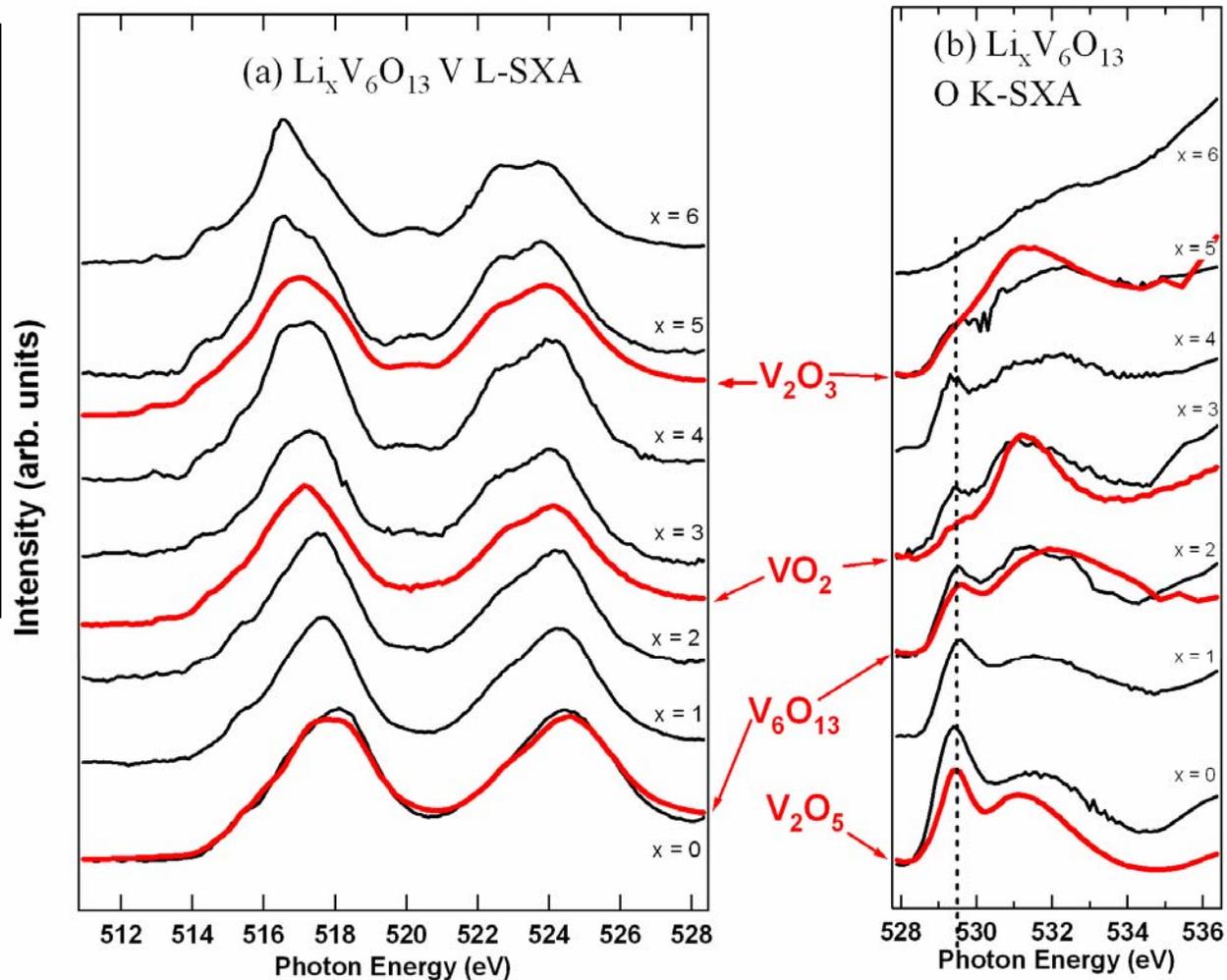
L.-C. Duda, T. Schmitt et al., Phys. Rev. Lett., Comment (2004)

Li insertion into V_6O_{13} battery cathodes



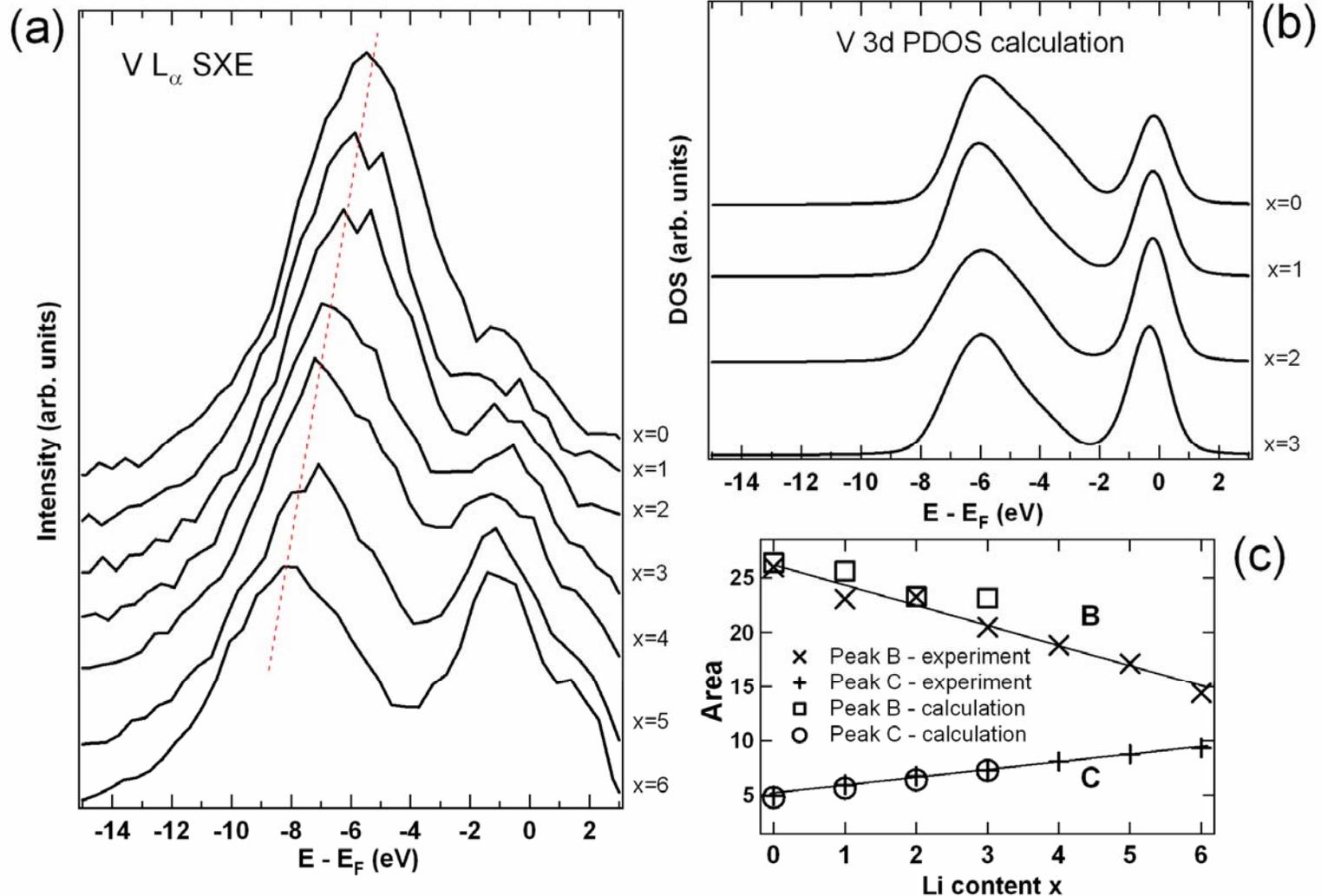
V L: V 2p \rightarrow V 3d

O K: O 1s \rightarrow O 2p



T. Schmitt et al., J. Appl. Phys. (2004)

SXE of $\text{Li}_x\text{V}_6\text{O}_{13}$

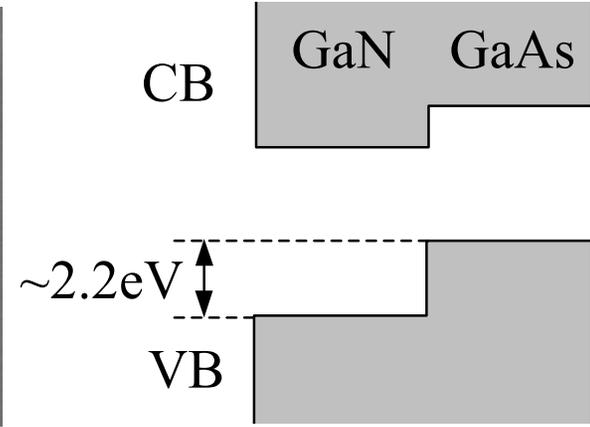
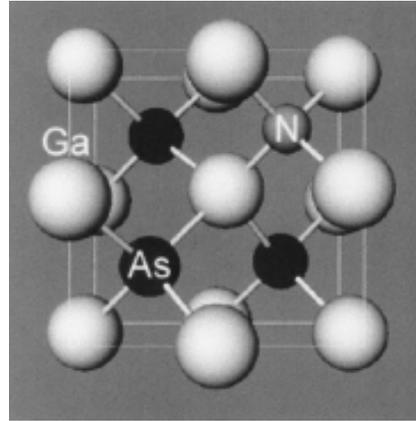
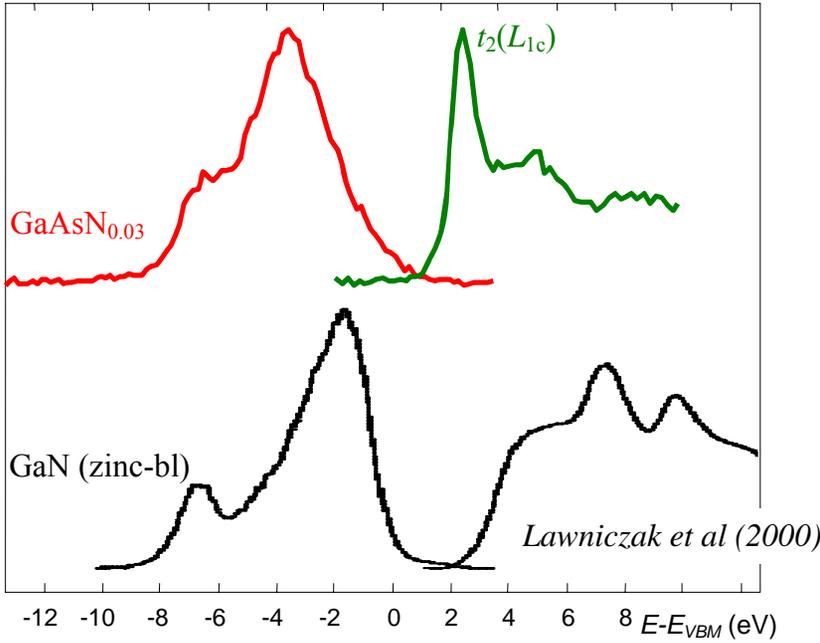


- quasi-rigid band behavior

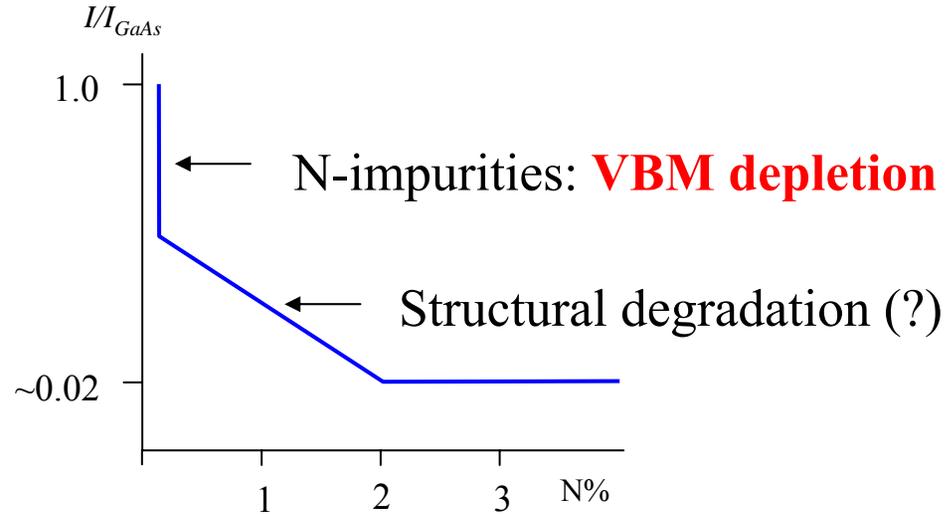
T. Schmitt et al., Appl. Phys. Lett. (2005)

Local nitrogen electronic structure of Ga(In)AsN

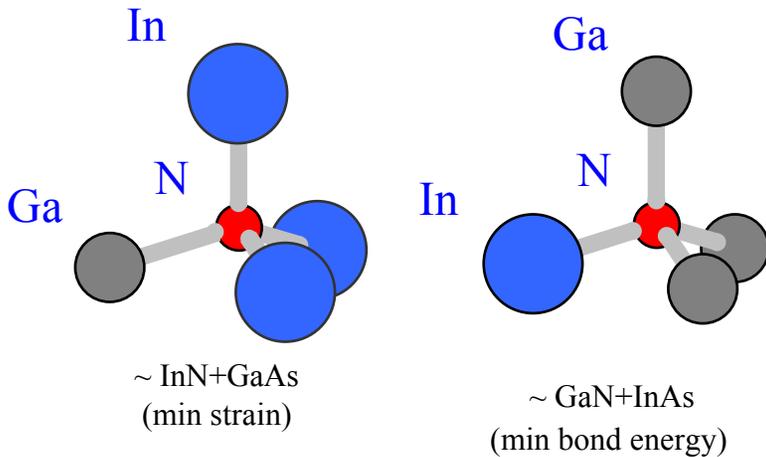
384 386 388 390 392 394 396 398 400 402 404 $h\nu$ (eV)



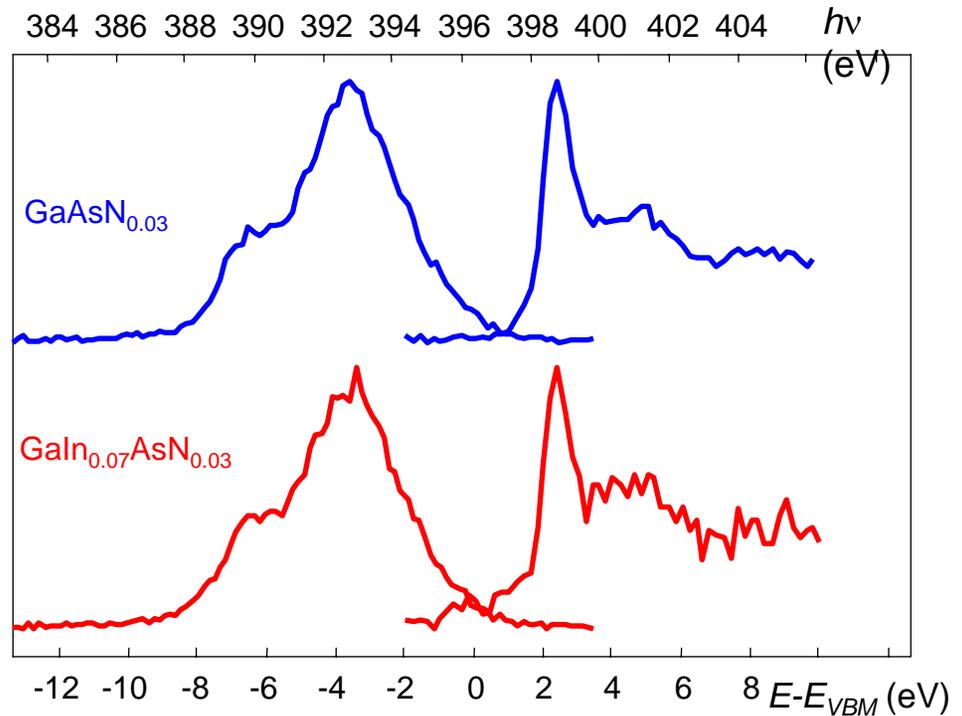
- Clear differences between GaAs:N and GaN in both VB and CB
- N-local charge depletion in VBM limits optical efficiency



Effects of In incorporation

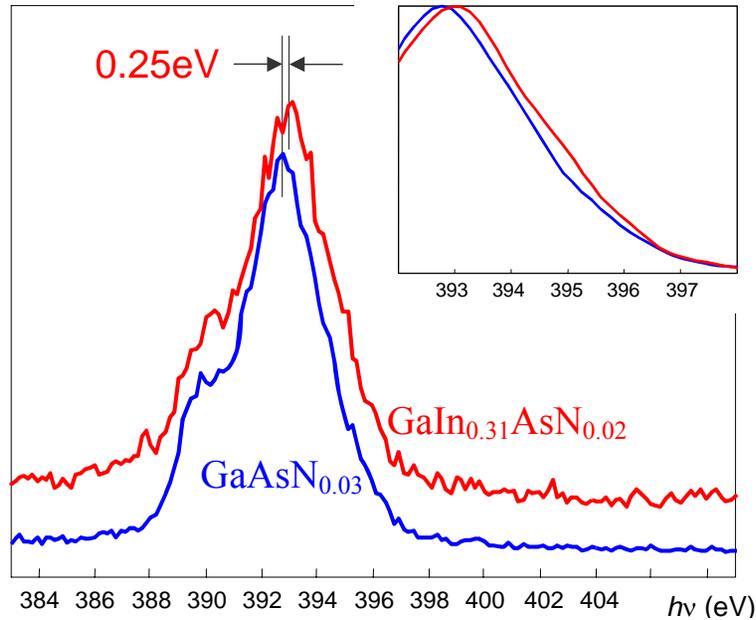


- No significant changes for low In content: In-depleted N local environments (Ga_4N , $\text{Ga}_3\text{In}_1\text{N}$)
- Optical efficiency increase due to better lattice match only

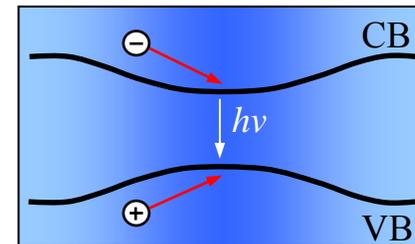
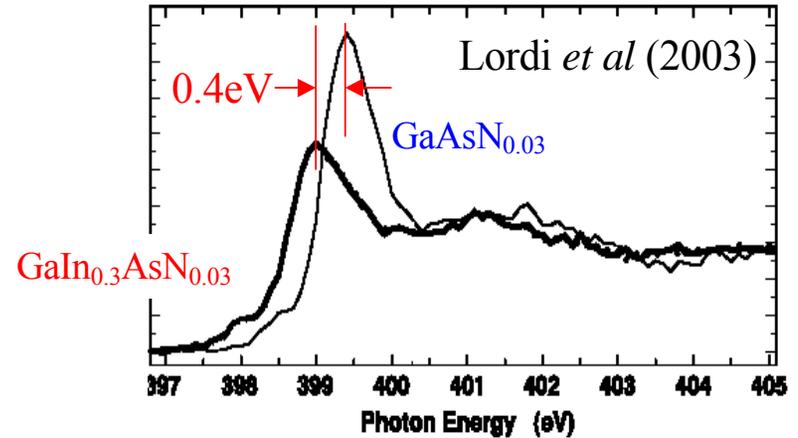


V.N. Strocov, P.O. Nilsson, T. Schmitt et al.,
Phys. Rev. B (2004)

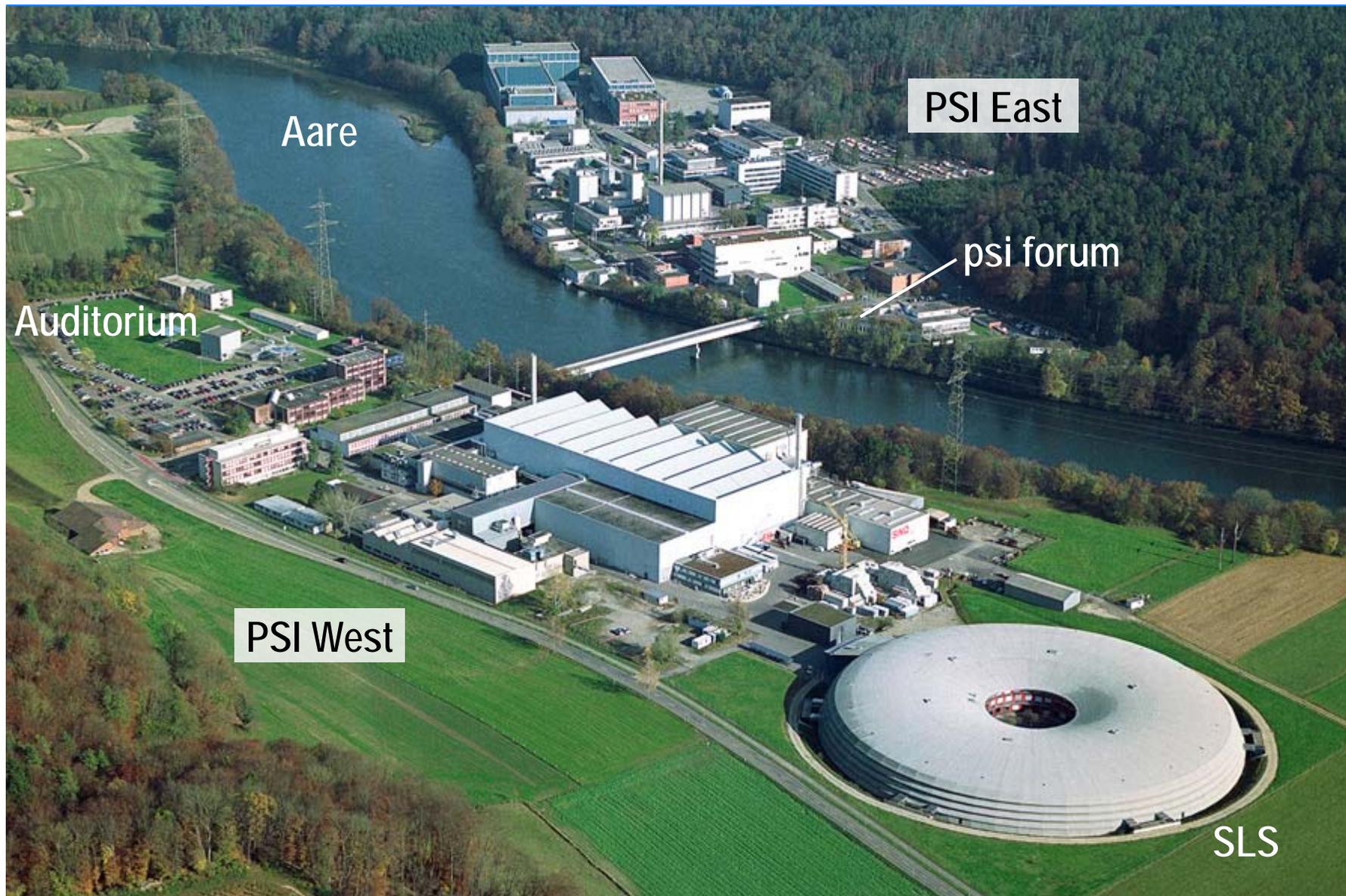
High In concentrations



V.N. Strocov, P.O. Nilsson, T. Schmitt et al.,
Phys. Rev. B (2004)



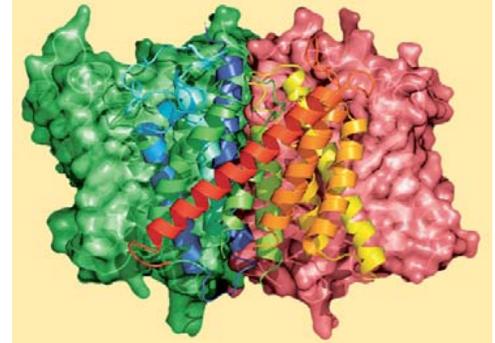
- In-rich N local environments (In_4N , GaIn_3N) result in VB and CB shifts towards each other
- ⇒ optical efficiency increase due to carrier confinement



Swiss Light Source SLS



Giant microscope for structure determination



Decoded by synchrotron light: AmtB membrane protein, enables the transport of ammonia (nutritive substance) to the plants.

Scientific goals

- Investigating the electronic structure of materials showing superconductivity, CMR, metal-insulator transitions, ferromagnetic, novel semiconducting and diluted/nanostructured materials ... with X-ray spectroscopy

- beamline with $h\nu$ range 400-1800 eV (K -edge of N, L -edges of Ga, Ge, As and most TMs, M -edges of REs ...)

- RIXS spectrometer with $E/\Delta E \sim 13000$ @ 1000 eV

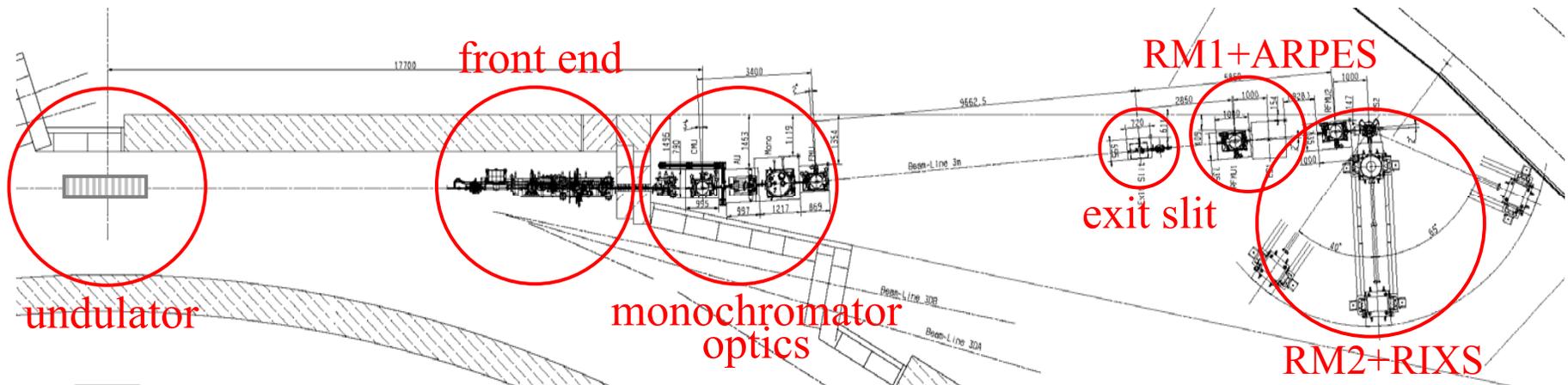
- variable scattering angle to study the q -dependences in RIXS: X-ray spectrometer on rotating platform

- ARPES station for k -resolved electronic structure

1																	2
3	4											5	6	7	8	9	10
11	12											13	14	15	16	17	18
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
87	88	89	104	105	106	107	108	109	110								
		58	59	60	61	62	63	64	65	66	67	68	69	70	71		
		90	91	92	93	94	95	96	97	98	99	100	101	102	103		

ADvanced RESonant Spectroscopy (ADDRESS) beamline @ SLS

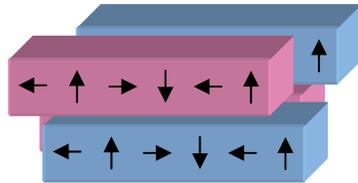
- undulator BL
- soft-X-ray radiation with variable polarization
- energy range 400 – 1800 eV
- resolving power $E/\Delta E \sim 28\,000$ @ 1 keV
- RIXS (and ARPES) endstations



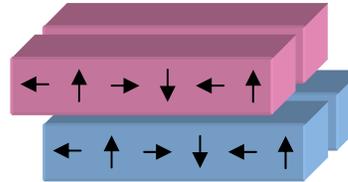
Undulator

Apple II-type undulator with fixed gap

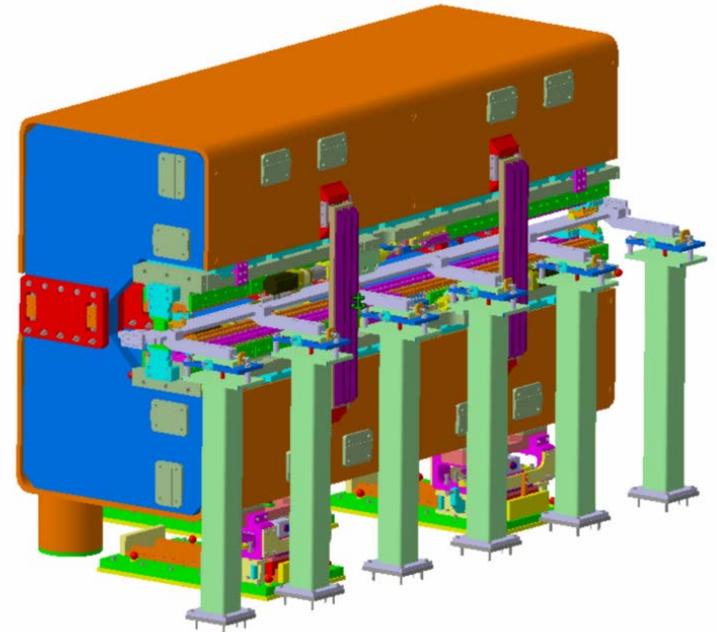
P-shift



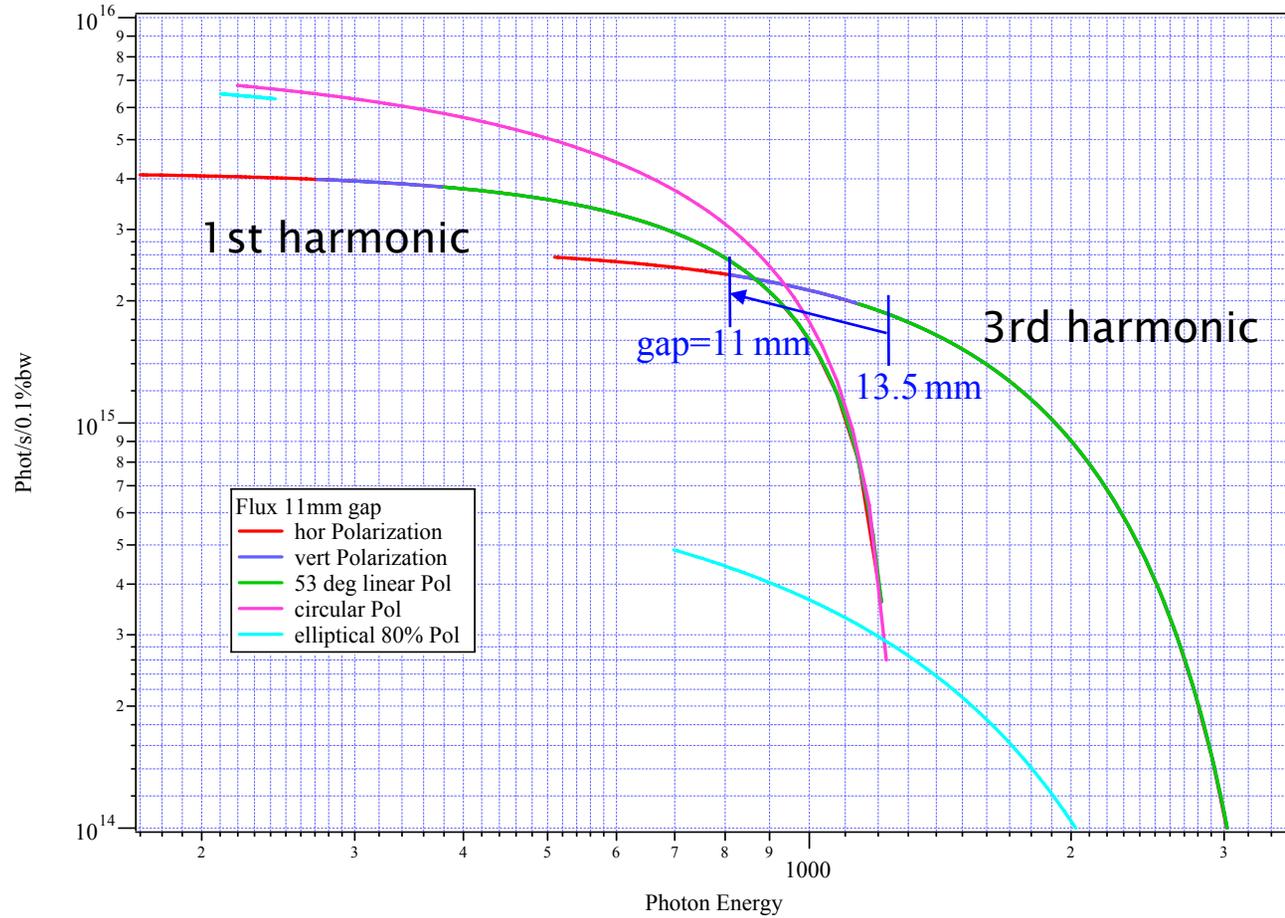
E-shift



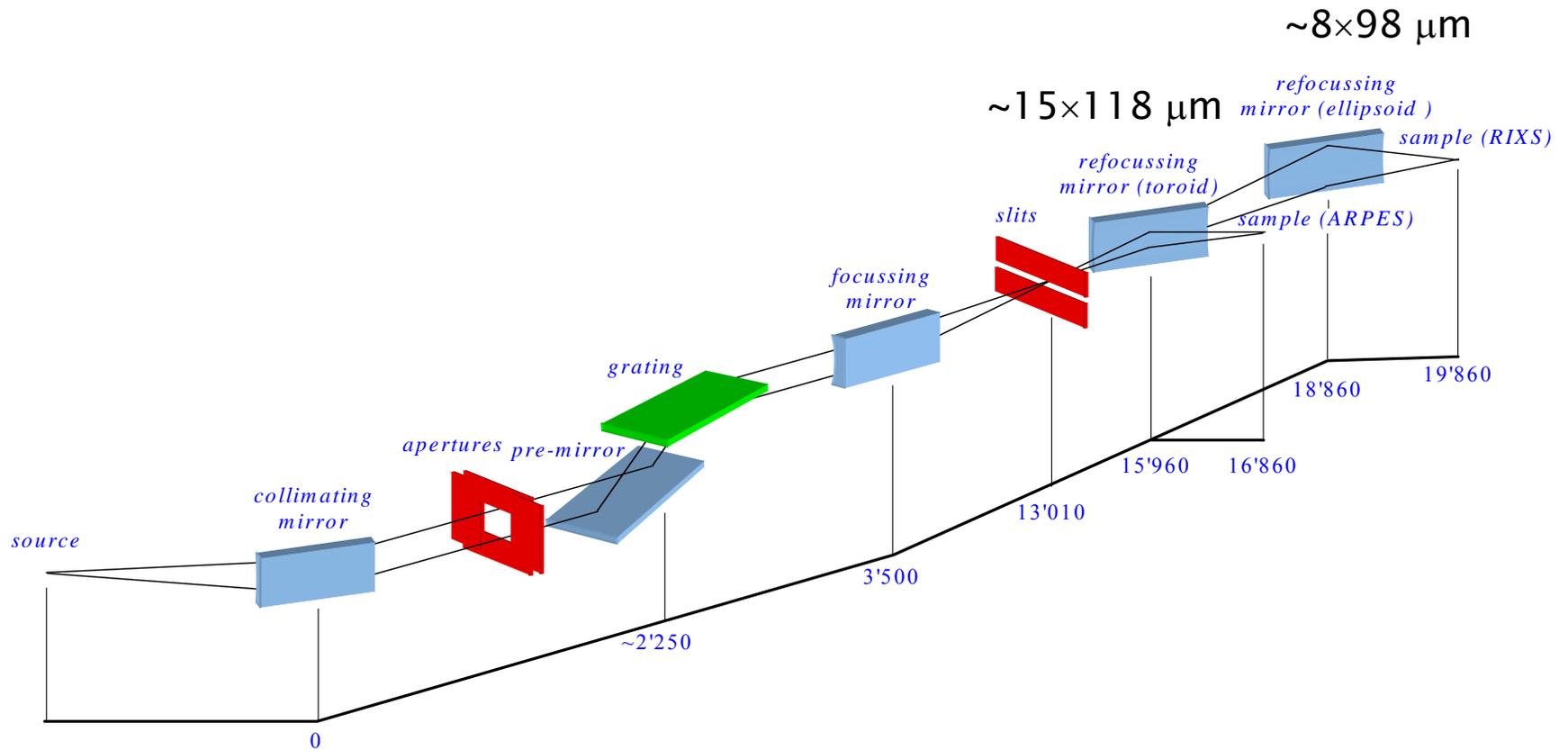
- variable polarization
 - fixed gap = 11 mm
 - period length = 44 mm
- optimized for $h\nu = 400\text{--}1800$ eV
- number of magnet pairs: $N = 7$
 - length of undulator: $L = 3.5$ m



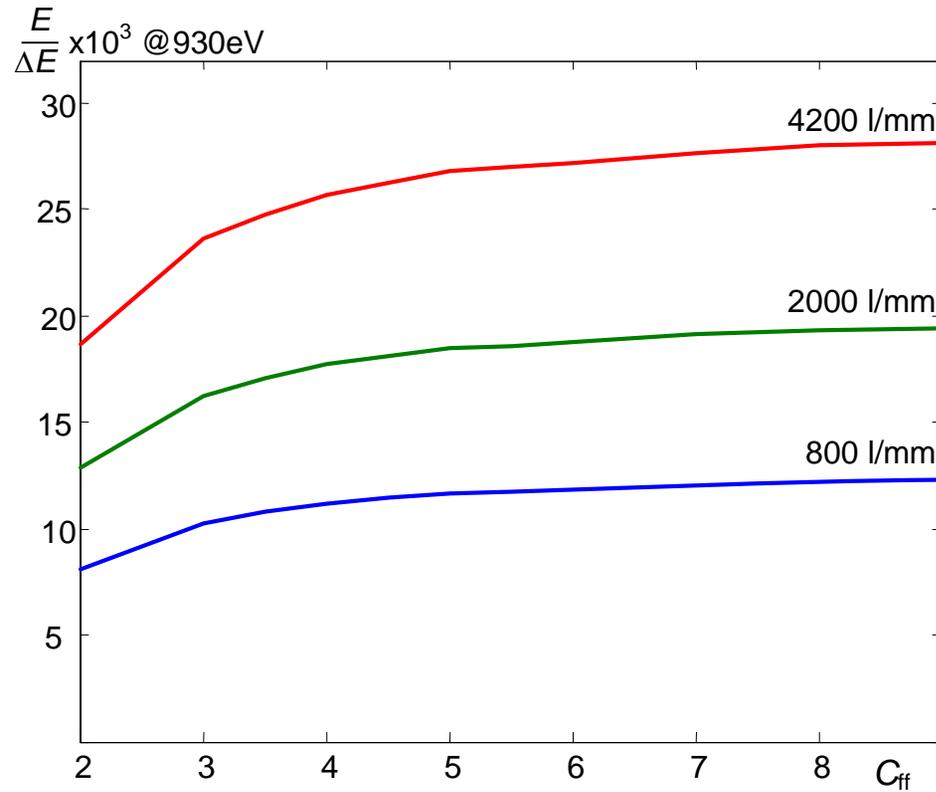
Predicted performance of the undulator



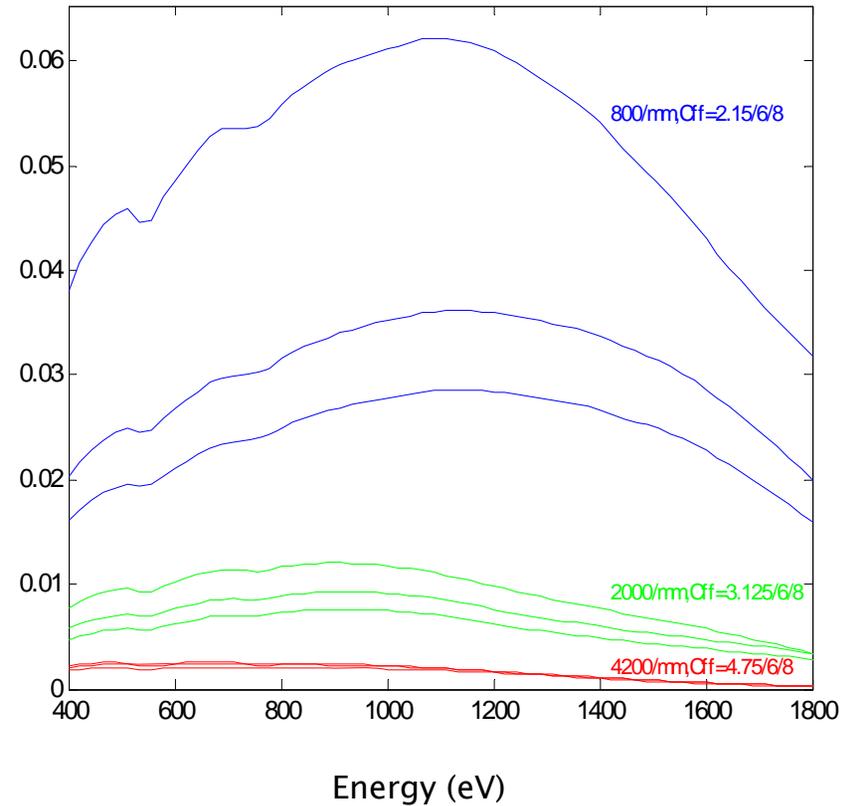
Optical scheme: Collimated-light PGM



Monochromator gratings



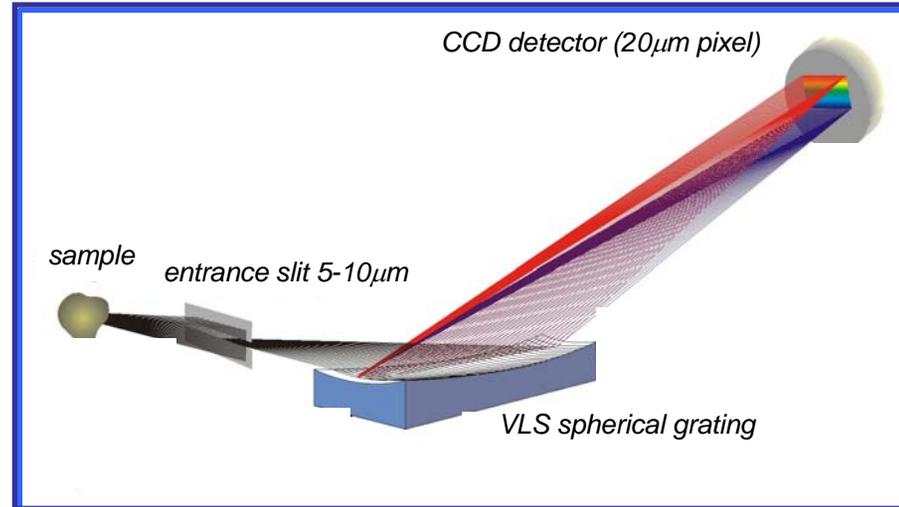
Beamline transmission



- Politecnico di Milano (L. Braicovich, C. Dallerà, G. Ghiringhelli);
EPFL Lausanne (M. Grioni)

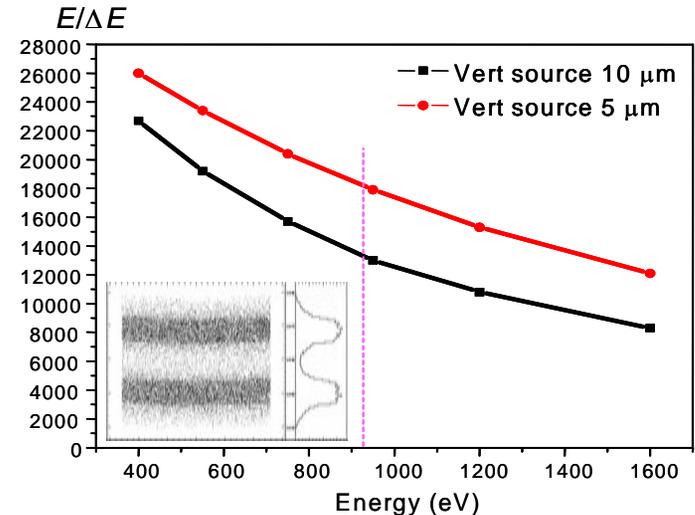
- Optical scheme

- Spherical VLS grating 3200 l/mm
- CCD detector
- dispersion arm ~4 m

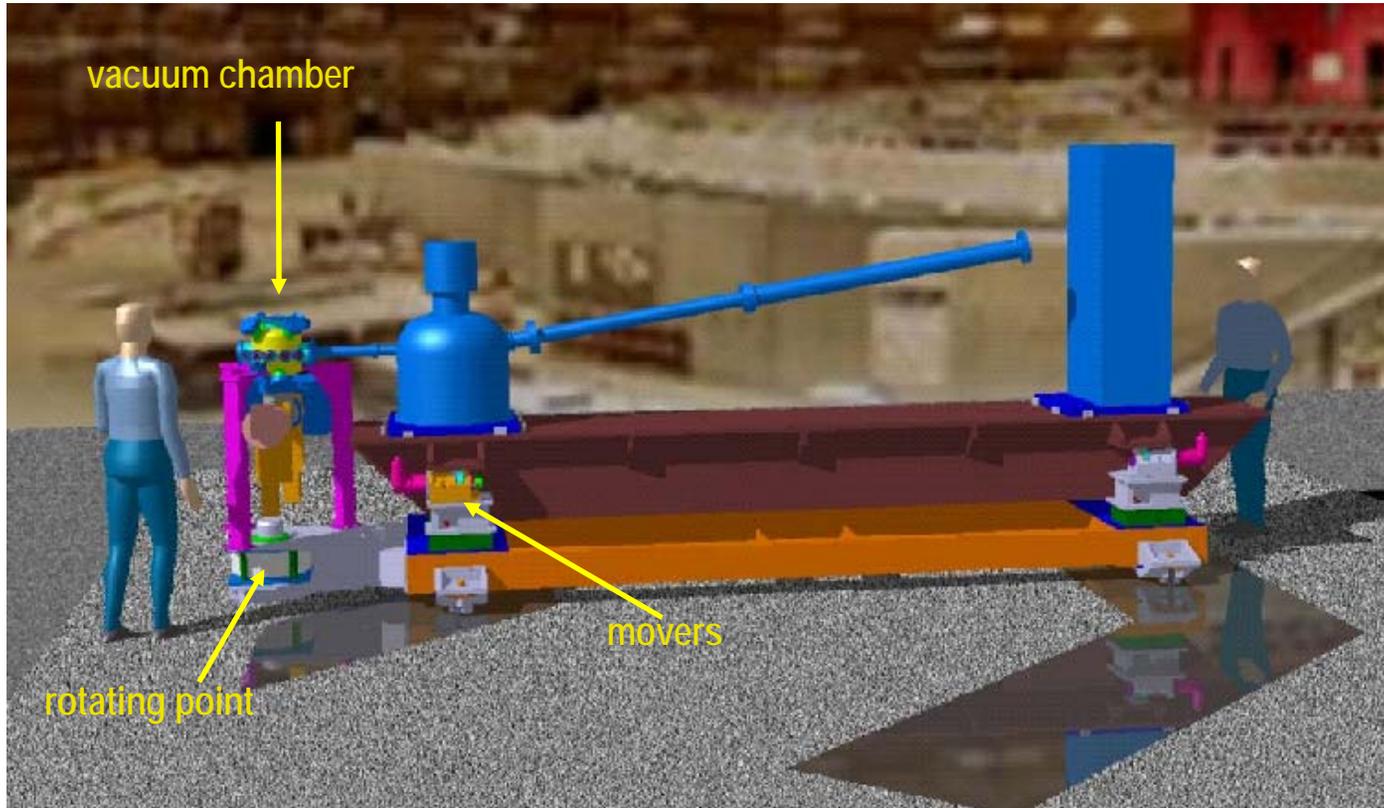


- Ray tracing calculations

- $E/\Delta E \sim 13000$ eV @ 1000 eV
- spot size <math><10 \mu\text{m}</math> for slitless operation



q-platform

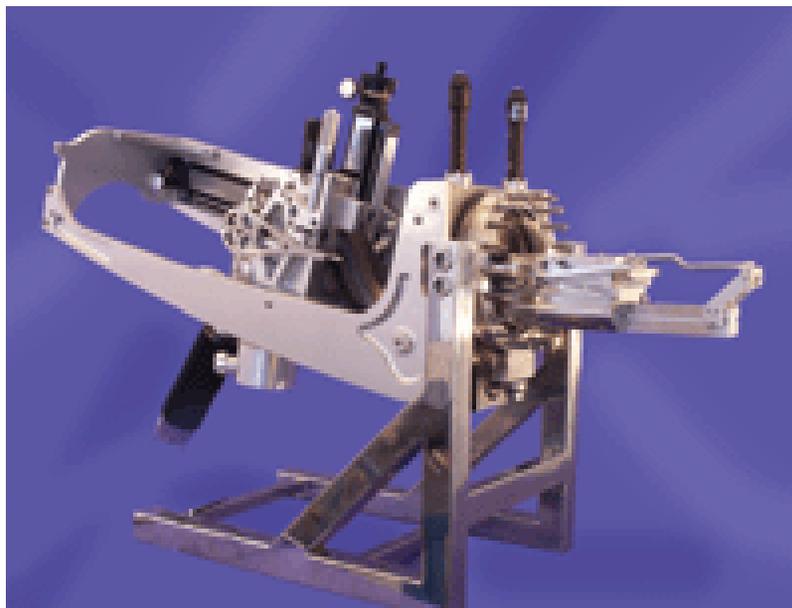


- variable scattering angle to study the q -dependences:
X-ray spectrometer on rotating platform
- rotation range 25-130° in the scattering angle
- air cushions

Scientia XES 350

- Nordgren-type Scientia XES 350 spectrometer at ARPES-port
- Alternative for diluted materials needing high through-put at moderate resolution

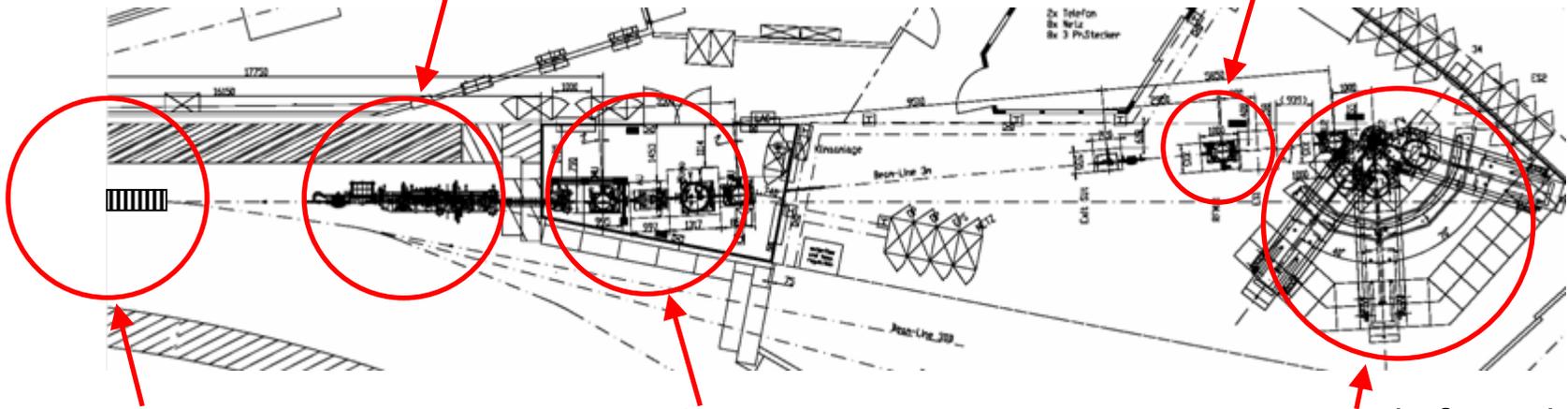
$$E/\Delta E \sim 2000$$



Milestones of ADRESS

Front end: Ordered, January–
installation March 2006

ARPES port: Conceptual design for ARPES endstation – port will be equipped with a Scienta XES 350 spectrometer first



Undulator: Magnet arrays in assembly, mechanics installation by June 2006

Optics: Monochromator, mirrors and gratings delivered; vacuum chambers and mechanics ordered; installation by April 2006

RIXS endstation: Platform delivered; spectrometer in assembly (Milano); installation by March 2006

First light and begin of commissioning for end of 2006



Summar y

- **Vanadium oxides: Localized (low energy excitations) and delocalized (ordinary fluorescence) contributions in the RIXS spectra**
→ higher resolving power needed
- **Local electronic structure of diluted semiconductors (GaInAsN)**
- **ADRESS beamline at SLS: Studies of q-dependence**

